A Quantum Computation Will Lead to the Discovery of a New Drug in the Next Decade

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I. ABSTRACT

The proposition that a quantum computation will lead to the discovery of a new drug within the next decade is motivated by the limitations of classical drug discovery methods and the potential of quantum computers to perform chemically accurate simulations of molecular systems. Those in favor of this claim argue that fault-tolerant quantum algorithms, particularly quantum phase estimation, provide the possibility of offering precise calculations of ground-state energies and binding affinities. Ultimately, reducing the early-stage candidate screenings reduces the need to test tens of thousands of compounds. Classical methods often fall short in accurately modeling systems with various interacting electrons. Advances in quantum algorithms, such as qubitization and quantum signal processing, demonstrate a plausible pipeline toward achieving chemically accurate simulations on quantum hardware. Those against these claims counter that extending these methods to large-scale and or drug-relevant systems requires deeply coherent circuits, large logical qubit counts, and large fault-tolerance overhead. As a result, placing the required physical qubit numbers and gate depths becomes far beyond current and future hardware capabilities. Rapid scaling of Hilbert space dimension, runtime, and noise accumulation in combination with decoherence limits feasibility. After considering both perspectives, the class ultimately favored the opposing view, with a 6-3 vote against the proposition.

II. INTRODUCTION

Drug Discovery is the scientific process of identifying novel molecules capable of modifying biological functions to treat diseases. Drug discovery can be a lengthy process using classical methods, often taking around 13 years and costs can reach 1.3 billion dollars per drug approved[1]. Since production of these drugs is so costly, only a few drugs are approved each year. In 2020, only 53 drugs were approved by the FDA[6]. This cost and time of developing drugs stem from classical methods not being able to accurately model molecular interactions between different compounds.

Classical models fail to compute how molecules interact with the level of precision needed to be useful in quantum chemistry[11], thus researchers need to produce 10,000s of potential candidates for a drug. These tens of thousands of candidates need to all go through preclinical and clinical testing, which leads to the vast majority failing to produce a viable drug[1]. If the candidates could be modeled accurately before preclinical trials, then drug failure rates would go down, reducing costs and time.

III. TECHNICAL BACKGROUND

This discovery process occurs in 4 main stages. The first is the target identification, where researchers find a biological molecule linked with the medical condition, such as a protein or a gene. Once a target is found, researchers will then look at tens of thousands of potential compounds that could bind to or affect the protein. These hits will be the starting point where researchers look for an effective drug. After hit discovery, the potential candidates are improved with lead optimization to improve their binding affinity and stability. Finally, researchers take these candidates and run them through years of preclinical and clinical testing, hopefully leading to one of these candidates being approved by the FDA to be used by patients. To be able to accurately model molecular interactions, researchers would need to use quantum chemistry to simulate the quantum mechanics of atoms. Quantum chemistry is the process of computing the behavior of electrons in atoms and molecules using the laws of quantum mechanics. Being able to calculate how electrons behave is important because this allows for the calculation of the binding affinity between molecules, which will allow for drugs to be discovered that are more effective. Classical models fail at calculating this because computation past 100 electrons becomes infeasible[11], which means that any simulation done on a classical computer will either be too inaccurate to be useful[11], or not have enough electrons to simulate a molecule that would be useful in drug discovery.

Quantum computation, on the other hand, could be useful in performing quantum chemistry. Quantum chemistry needs precise calculations of energy states to model a stable molecule. These energy states can be calculated using quantum phase estimation to solve the electronic Schrodinger's Equation $e^{-iHt}\left|\psi\right\rangle = e^{-iE_n t}\left|\psi\right\rangle$ where H is the electronic Hamiltonian, $|\psi\rangle$ is the molecular wave function, and E_n is the energy state corresponding to that state. If researchers can compute E, then we can model a molecule's ground state, predict its stability, and understand how it will interact with other molecules. Quantum phase estimation is the process of calculating theeigenvaluee given a unitary U, and an eigenstate $|u>$ such tha, $U|u>= e^{i2piphi}|u>$. Quantum phase estimation will be able to accurately estimate phi up to n bits

,where n is the size of the register that will hold phi. The workflow of QPE works like this(See figure 1 and 2 for an illustration). First, there will be 2 registers initialize to $|0\ldots0\rangle$(we will call this register 1) and $|u\rangle$(register 2). Then, register one is put through Hadamard gates to create a superposition and then both registers are used to apply U^{2^k}, where k is the index of the qubit in register 1 that will be used as the control bit. Lastly, an inverse Fourier transform is applied to register 1 and the register is measured. What will come out of the register are the bits of phi that can be used to find the eigenstatee above. Since this eigenstate can be solved, then the eigenstate can be used to find E_n, which is the ground state.

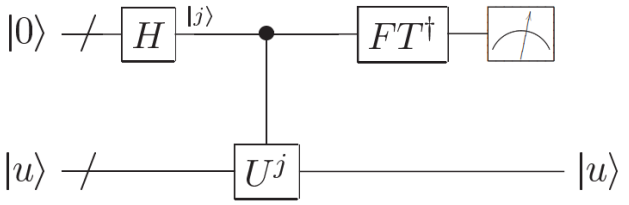

Figure 1: The Quantum Phase Estimation Ciruit[8]

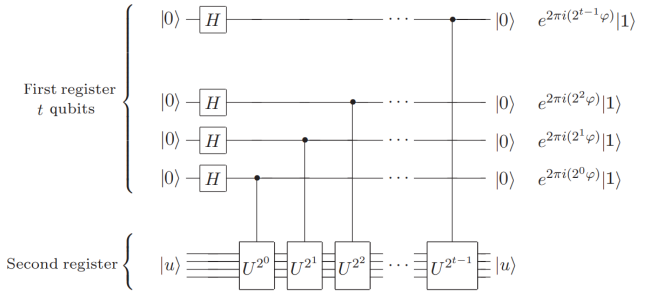

Figure 2: The first 2 steps of QPE[8]

IV. THE CASE FOR

The case for this is simple, if quantum phase estimation is solved within the next decade, then researchers will have the necessary tools to perform accurate quantum chemistry to help simulate their candidates and find a suitable drug before going through years of clinical testing.

To understand a base line for what would be the resource requirements needed to use quantum phase estimation as an accuracy needed for drug development, we looked a study conducted by Reiher et al 2017[8] that provided a basis for what a fault tolerant computer would need to calculate a chemically accurate ground state. For a chemically accurate calculation of an energy state, the estimate will need to be within 1 milli hartree, or about $4.3597 * 10^-22$ joules.

For a theoretical molecule, Reiher chose to use two different structures of FeMoco as models for a sufficiently complex drug[8].3 Different models for algorithms were used to perform QPE on these 2 structure. The first model was a fully serial execution where each Hamiltonion evolution would be executed one after another to minimize the amount of qubits needed to run the calculation. The second model, programmable ancilla rotations(PAR), would calculate the necessary rotations in parallel factories before hand and then teleport them into the circuit when needed. The third model(Nesting) would calculate would execute Hamiltonian terms that affect disjoint sets of spin orbitals in parallel. All three models offer different approaches to solving QPE while emphasizing different priorities such as time and space complexity.

This study gave different resource estimates on each of the 3 models. For the Serial model, emphasis was given on limiting the amount of needed logical qubits, and this was reflected with the amount of logical qubits being only around 111 for structure 1 and 117 for structure 2. The limiting of qubits comes at a cost, however, with each structure taking 130 and 240 days to calculate. The estimated amount of T and Clifford gates were high, with order 10^{15} of each gate needed for both structures. For PAR, time was emphasized, and therefore the time it takes was significantly reduced to 110 hours for structure 1 and 210 hours for structure 2. The tradeoff, however, was a significant spike in logical qubits to needing around 2000 for both structures. The amount of T and Clifford gates also jumped, needing about 10^{16} magnitude of each gate to run[8].

Although Reiher did offer a good base line for how much a potential QPE algorithm may cost, there were some areas where it can be improved. Reiher used traditional Lie-Trotter-Suzuki formulas to preform the time evolution of the Hamiltonian. The Trotter formula is: Let A and B be Hermitian operators, then for any real t: $\lim_{n\to\infty}(e^{iAt/n}e^{iBt/n})^n = e^{i(A+B)t}$. Trotter's formula uses a simple and easy to implement method of evolving the hermitian, but since it only works for large r, many steps are required to give a sufficient evolution[16]. A large amount of steps requires a large amount of gates, and more gates lead to more noise from each gate. It is imperative to limit the amount of gates required to run QPE so that the final calculation is accurate enough to be chemically useful.

A study published in 2021 offers an alternate to trotter's formula that both limits the amount of gates needed and also limits the amount of time required[16]. Von Burg at al in 2021 published an alternative that uses qubitization and quantum signal processing in lieu of trotter's formula to evolve the Hamiltonian.

Qubitization is the process of embedding a Hamiltonian H inside a larger unitary walk operator W that will allow for polynomial transformations to be preformed on H. Von Burg defined W as $W = e^{i\sin^{-1}H/\alpha}$ where H is the hermitian and α is some normalizing constant $\alpha \geq ||H||$ to ensure that arcsine is real. This allows for W to be implemented exactly using single qubit rotations. After finding the phase $\phi = \sin^{-1}E_k/\alpha$, E_k can be found using a $\sin\phi$ classically[16]. This allows for phase estimation to happen without any trotterization error associated with

the old method. This also means that this calculation can happen with dramatically less gates. This algorithm used toffoli gates instead of T and Clifford gates (For reference a Toffoli gate can be implemented in 4 t gates[16]), but even with the new gate type the reduction in complexity is significant. Von Burg also preformed QPE on Femoco, and was able to reduce the Toffoli gate count to a magnitude of 10^{10} gates with a error of at most 1 milli hartree[16]. For reference, with trotterization, the same calculation at the same precision takes a magnitude of 10^{14} toffoli gates. It is important to note that the amount of qubits needed increased to around 3600, but even then that is not insurmountable within the decade. With qubitization and quantum signal processing, the amount of needed gates can be reduced from 10^{14} to 10^{10} Toffoli gates.

This is about where the theory is right now, but what about actual experimentation? Significant progress has already been made. Yamamoto et al in 2025[18] has already been able to conduct an experiment on Hydrogen to calculate the ground state using QPE. This study used a large encoded circuit that was able to successfully execute 7200 2 qubit gates to calculate the ground state within 1 milli Hartree, which would be chemically accurate. Additionally, this experiment ran with a [7,1,3] color code for quantum error correction[18]. They also used fault tolerant Clifford and Rz gates. Although this was a small molecule, Yamamoto was able to get experimentally chemically accurate precision, and this quantum error correction can be applied to larger momlecules as technology develops.

So, at least right now in theory, there is a reasonable need in qubits and a moderately high requirement for Toffoli gates. There have been improvements in how the algorithm works to massively reduce how many gates are needed, and as companies increase the amount of qubits, it should be possible for drug developers to have the necessary tools to discover a new drug in the next decade.

V. THE CASE AGAINST

The proposition that a quantum computer will lead to the discovery of a new drug within the next decade relies on the assumption that quantum computers will soon be capable of performing chemically accurate simulations of drug-scale molecules. This implicit assumption can be evaluated using a two-part validity test. As an initial condition, small benchmark molecules should already simulate with chemical accuracy on realistic quantum hardware. The second condition should demonstrate the scaling of those benchmark results to drug-relevant systems and prove feasible within a ten-year time-frame. At present, neither condition is sufficient to accomplish the ten-year time-frame for drug discovery .[4, 9, 12, 17]. .

A. Requirements for Drug-Scale Quantum Chemistry

Quantum chemistry simulation focuses on the ability to implement time evolution under the electronic Hamiltonian, which $\hat{H}$ encodes the electron-to-electron interactions, nuclear positions, and the kinetic energy terms terms [9, 17].

$$U(t) = e^{-i\hat{H}t}. \tag{1}$$

The focus of the simulation is to solve the corresponding eigenvalue problem, where eigenvalues E_k represent the quantized electronic energy levels of the molecular system. The difference between these energy levels determines molecular configurations, reactions, and binding.

$$\hat{H}|\psi_k\rangle = E_k|\psi_k\rangle. \tag{2}$$

the scope of molecular binding, either bound or unbound electronic states, energy differences become more favorable. When the energy difference between these electronic states is large and negative, the bound state would signify a lower point on the potential energy surface, producing a value energetically favorable and complex against thermal excitation. When thermal fluctuations are insufficient to overcome the binding energy, the result would indicate a strong affinity. In contrast, when the energy difference is near zero, bound and unbound states are nearly degenerate, and fluctuations can create weak binding. Small errors in electronic eigenvalue estimation can therefore alter the predicted binding behavior and emphasize the importance of near-accurate determinations of reaction barriers, molecular stability, and binding affinities for drug testing ... accomplish the ten-year time-frame for drug discovery [4, 9, 12, 17].

Quantum phase estimation (QPE) provides a mechanism for computing these energies by extracting the electronic eigenvalues E_k of the molecular Hamiltonian. Encoding each eigenvalue into a measurable quantum phase, QPE enables a direct estimation of the energies in these states.

$$\phi_k = \frac{E_k t}{2\pi}, \tag{3}$$

The algorithm encodes these phases, where t is the total simulated time evolution. Fine precision indicates that a longer simulation time yields a finer energy resolution [7, 9] .

$$\Delta E \lesssim 10^{-3}\,\text{Ha}. \tag{4}$$

To produce chemically meaningful predictions, energies must be contained within the threshold in Equation 4. Errors larger than the threshold would then indicate chemically unreliable values.

B. Exponential Scaling and Benchmark Limitations

The physical challenge inhibiting quantum chemistry arises from the exponential growth of the many-electron Hilbert space. For size N_e correlated electrons represented in a basis of size M spatial orbitals, the dimension scales combinatorial as

$$\dim \mathcal{H} = \binom{2M}{N_e} \tag{5}$$

reflects the number of fermion configurations [17]. As a result, chemically realistic molecules with dozens of correlated electrons correspond to Hilbert spaces of large dimensions. Indicating, molecules with N_e 50-100 correlated electrons span a Hilbert space of 10^{15}–10^{30} configurations in orbital spaces [4, 17] . This is emphasized to illustrate that benchmarks are theoretical scaling exercises but span beyond hardware capabilities.

C. Benchmark Scaling and Gate Count

At a benchmark scale, quantum chemistry is already challenging. The FeMoco molecule is often cited as a representative case, yet practical simulations utilize 14 correlated electrons for an active space [9, 12] . Despite aggressive truncation, fault-tolerant simulations are estimated to require

$$G_{\text{bench}} \approx 2.4 \times 10^9\text{–}10^{10} \tag{6}$$

logical gates and several thousand logical qubits [12]. To evaluate where such benchmarks translate to authentic drug-relevant systems, consider this hypothetical scaling argument based on established trends reported by Rocca et al.[12]. Their analysis suggests that logical gate counts scale with electron number, approximately as

$$G \propto N_e^4, \tag{7}$$

reflecting the growth of the Hamiltonian norms and qubitization costs with system size [4, 9, 12] . Extracting from the benchmark system, the 14 electrons in drug-relevant systems N_e 50-100. Below, f represents the scaling factor, where the numerator represents the typical size of drug relevant system's electrons over the benchmark resource. Substituting these values indicates a two-to-three order of magnitude increase in gate count from electron number scaling.

$$f = \left(\frac{N_{e,\text{drug}}}{N_{e,\text{bench}}}\right)^4 \approx \left(\frac{50\text{–}100}{14}\right)^4 \approx 10^2\text{–}10^3. \tag{8}$$

Applying this factor to the benchmark resource estimate yields

$$G_{\text{drug}} \approx f \cdot G_{\text{bench}} \approx (10^2\text{–}10^3)(2.4 \times 10^9) \approx 10^{11}\text{–}10^{12}. \tag{9}$$

With upper estimates approaching the magnitude of thirteen gates when tighter precision requirements or larger basis sets are considered. This hypothetical is not to constitute new resource estimations, but to illustrate how an established benchmark result can scale unfavorably when extending to drug-scale systems.

D. Hamiltonian Simulation Depth and Precision Limits

Equation (6) demonstrates the depth precision relationship in QPE, where the change of energy requires a number of controlled time evolution operations scaling as

$$N_U \sim \mathcal{O}\left(\frac{t}{\Delta E}\right) \tag{10}$$

[9]. Ni et al. analyzed proposed low-depth variants of phase estimation and indicated that the circuit depth reductions are achieved only by relaxing the energy precision, not by the scaling of $\frac{1}{\Delta E}$[7] . When chemical accuracy is preferred, these low-depth methods recover the same asymptotic depth scaling as standard QPE, implying that shallow circuits do not suggest accurate Hamiltonian circuits [7, 9] . In other words, at high precision, the circuit depth grows with the same dependence on the target energy change.

E. Decoherence, Noise and Fidelity

Quantum hardware is imperfect, because qubits are not perfectly isolated from their environment. As a result of these flaws, decoherence refers to the loss of quantum phase information due to uncontrolled interactions with the surroundings. This is encompassed by random errors introduced during gate operations and measurements. All combined, these effects limit how long quantum information can be stored and manipulated.
Each physical quantum gate fails with some probability p, which is small, and is unavoidable in even the most recent devices. For a quantum circuit containing G gates, the probability of no errors occurring in the computation is approximately

$$(1-p)^G \approx e^{-pG} \tag{11}$$

This defines circuit fidelity,

$$F \approx e^{-pG} \tag{12}$$

Which measures the likelihood that the final quantum state remains correct. The exponential dependency on gate count is essential, and more so when considering low per-gate error rates that hover around near failure when the circuit depth becomes too large. If we were to consider the hypothetical, this would indicate that the fidelity rapidly approaches zero. Overall, indicating the

quantum state loses its encoded information before the computation can complete.

Some experimental studies of superconducting qubits report coherence and relaxation times in the order of milliseconds [13, 15] . Although this supports experimental success, there are many orders of magnitude shorter than what would be required to perform chemically accurate QPE circuits of the required depth. This would result in fidelity collapse and make deep quantum chemistry algorithms difficult with noisy-intermediate-scale-quantum (NISQ) devices [10]. To overcome decoherence, fault tolerance is required. Surface code error correction requires thousands of physical qubits per logical qubit, depending on target error rates and circuit depth [3, 5, 10].
When drug scale quantum chemistry requires 100 logical qubits, this implies a total physical qubit requirement of

$$N_{\text{phys}} \gtrsim 10^5\text{–}10^6 \tag{13}$$

Current quantum processors contain roughly 1000 physical qubits, and more optimistic projections fall short by at least an order of magnitude [10].

Quantum processors implement limited qubit connectivity, and the use of SWAP operations enables interactions between nonadjacent qubits. $G_{\text{total}} = G_{\text{alg}} + G_{\text{SWAP}}$,where the routing overhead increases along with the system size, represents the total depth and overall routing overhead. This expression G_{alg} represents the the algorthimic gate count under connectivity in addition to G_{SWAP} accounting for gates to route quantum information between the nonadjacent qubits. Cohen et al. and Litinski demonstrate that such routing overhead can persist in fault-tolerant surface code architectures[3, 5].

When considering simulations that require gates with magnitudes of eleven to thirteen [12], this would indicate an accumulation of higher error probability.

F. Scaling Barriers Beyond Benchmark Systems

These considerations indicate the technical and practical limits of current term quantum computing for drug discovery. Considering all the requirements for a chemically accurate quantum computation, the order of logical gates 10^{11}-10^{13} and 10^5-10^6 physical qubits contrasts with the current quantum hardware [3, 4, 7, 9, 10, 12, 13, 15, 17]. The feasibility of this claim would also have to consider the 10-15 year timelines of drug development [2, 14]. This gap provides a basis for the discussion of the proposition succeeding in the next decade.

VI. THE CLASS DISCUSSION

Class discussion primarily focused on evaluating the likelihood of the proposition within the next decade by contrasting the theoretical promise of quantum computing against practical and physical limitations. Arguments in favor emphasized the framework for simulating quantum mechanical systems and quantum phase estimation as critical for predicting chemical accuracy, molecular stability, and binding affinity. Participants mentioned the algorithmic advances, such as qubitization and quantum signal processing, all of which aim to reduce simulation error and improve efficiency by avoiding Trotterization. The discussion also noted experimental demonstrations of error-corrected quantum phase estimation on small molecules that achieved accuracy in large, fault-tolerant quantum circuits.

These results provided evidence that error correction can be stabilized under deep quantum circuits. In contrast, those opposing stressed that the methods to create realistic drug systems would require large circuit depths and substantial fault tolerance overhead. As a result of these implications, severe coherence and noise challenges can potentially remain. The discussion emphasized the rapid scaling from benchmark molecules to realistic drug candidates, all of which contribute to large logical qubit counts and computational complexity. The class weighed both perspectives and found the opposing side more consistent with current technological limits. The final vote was 6-3 against the proposition.

VII. CONCLUSIONS

This paper examined the proposition that a quantum computation will lead to the discovery of a new drug within the next decade by considering the advantages offered by quantum chemistry and the limitations affected by current quantum technology. Although quantum algorithms provide an important framework for modeling molecular systems, the resource requirements for feasible drug-scale simulation remain beyond the near-term capabilities. Deep circuit depths, large qubit counts, and significant fault-tolerance overhead bring up major difficulties. Advances in molecular simulations do not exclusively address the biological complexity and clinical testing stages that dominate drug development timelines. With all sides being considered, quantum computing has the capability of transforming quantum chemistry, yet unlikely to directly lead to a new drug discovery in the next decade under current assumptions. However, the steady pace of improving quantum technologies cautions overt optimism; we welcome future developments that may overturn this assessment.

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